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Application of X-ray Absorption Spectroscopy and Inelastic X-ray Scattering Techniques to Study Lithium Ion Battery Materials

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Lithium ion batteries have attracted worldwide attention in the past decades due to their high energy and power density. They are currently widely used in portable devices and power tools and are poised for use in vehicular applications. It is important to understand the redox mechanism from a fundamental point of view to help develop new battery materials with improved properties. Various techniques such as nuclear magnetic resonance, conventional diffraction, short-range and long-range x-ray probes, Mössbauer spectroscopy, x-ray absorption fine structure, electron energy loss spectroscopy, etc. have been employed to date. The interesting redox chemistry occurs at light elements (Li, O, C) and TM 3d orbitals during Li-ion de/intercalation. We use x-ray absorption spectroscopy (XAS) and inelastic x-ray scattering (IXS) techniques to understand the charge compensation mechanism in operating batteries. The technique of XAS has been used to probe the local atomic and electronic structure details around specific probe atoms and provide key information on metal oxidation states and site symmetry. Using hard x-ray non-resonant IXS, which is a photon in/photon out technique, we demonstrate the ability to obtain truly bulk sensitive soft x-ray absorption—like information under normal battery operating conditions. The appropriate edge spectra of low-Z elements as well as metal were obtained using the lower-energy-resolution inelastic x-ray scattering spectrometer [1]. Recent studies of charge compensation in battery materials using XAS in Li_5FeO_4 [2] and IXS in $LiCoO_2$ will be presented.

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2. C. S. Johnson, S. H. Kang, J. T. Vaughey, S. V. Pol, M. Balasubramanian, and M. M. Thackeray, "Li_2O removal from Li_5FeO_4: A Cathode precursor for Lithium-Ion Batteries," *Chem Mater.*, **22**, 1263, (2010).